Multipartite Entanglement Signature of Quantum Phase Transitions

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We derive a general relation between the non-analyticities of the ground state energy and those of a subclass of the *multipartite* generalized global entanglement (GGE) measure defined by T. R. de Oliveira *et al.* [Phys. Rev. A **73**, 010305(R) (2006)] for many-particle systems. We show that GGE signals both a critical point location and the order of a quantum phase transition (QPT). We also show that GGE allows us to study the relation between multipartite entanglement and QPTs, suggesting that multipartite but not bipartite entanglement is favored at the critical point. Finally, using GGE we were able, at a second order QPT, to define a diverging entanglement length (EL) in terms of the usual correlation length. We exemplify this with the XY spin-1/2 chain and show that the EL is half the correlation length.

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Quantum Phase Transitions (QPTs) occur at zero temperature and are characterized by non-analytical changes in the physical properties of the ground state of a many-body system governed by the variation of a parameter λ of the system's Hamiltonian $H(\lambda)$. These changes are driven solely by quantum fluctuations and are usually characterized by the appearance of a non-zero order parameter [1]. Since QPTs occur at $T = 0$, the emerging correlations have a purely quantum origin. Therefore, it is reasonable to conjecture that entanglement is a crucial ingredient for the occurrence of QPTs (e.g. Refs. [2, 3, 5, 6] and references therein). If this is true, then the QPT would imprint its signature on the behavior of an entanglement measure. Under a set of reasonable general assumptions, Wu *et al.* [7] have demonstrated that a discontinuity in a *bipartite* entanglement measure (concurrence [10] and negativity [11]) is a necessary and sufficient indicator of a first order quantum phase transition (1QPT), the latter being characterized by a discontinuity in the first derivative of the ground state energy. Furthermore, they have shown that a discontinuity or a divergence in the first derivative of the same measure (assuming it is continuous) is a necessary and sufficient indicator of a second order QPT (2QPT), which is characterized by a discontinuity or a divergence of the second derivative of the ground state energy. Nevertheless, most of the models of 2QPTs considered so far did not present any *long-range* bipartite entanglement at the critical point, even though the correlation length diverges. Moreover, contrary to expectations, most of the measures discussed in the literature are, to the best of our knowledge, not maximal at the critical point, the exceptions being the one-site von Neumann entropy of the Ising chain [3], the localizable entanglement of a finite Ising chain with 14 sites [12], and some classes of the Generalized Global Entanglement (GGE) for the Ising chain [6].

In this Letter we firstly extend Wu *et al.* [7] results to a *multipartite* entanglement (ME) measure [8, 9], the GGE introduced in Refs. [6, 13], and discuss how non-analyticities in the energy are signaled by the GGE. Secondly, we define an entanglement length (EL) for an arbitrary collection of two-level systems. In the case of a symmetry-breaking 2QPT, this EL diverges at the critical point and is simply related to the correlation length. This result indicates that ME is most favored at that point, contrary to bipartite entanglement [2, 3, 4]. We consider the consequences of this result for specific spin-1/2 models presenting 1QPT or 2QPT.

In particular, for the 2QPT of the one-dimensional transverse field XY model we obtain all the relevant critical exponents, with the EL defined in terms of correlation functions (CFs) appearing in the GGE. We also show in this specific case that the GGE is maximal at the critical point, thus signaling the QPT, as three of us had already observed in the Ising case [6]. This last result, together with a diverging ME length at the critical point, reinforces that ME plays a significant role in QPTs.

Following Ref. [7], a discontinuity in (discontinuity in or divergence of the first derivative of) the concurrence or negativity is both necessary and sufficient to signal a 1QPT (2QPT) for systems of distinguishable particles governed by up to two-body Hamiltonians. The energy per particle (ε) derivatives depend on the two-particle density matrix elements as [7]

$$\partial_\lambda \varepsilon \;=\; (1/N)\sum_{ij} Tr\left[\left(\partial_\lambda U\left(i,j\right)\right)\rho_{ij}\right], \tag{1}$$

$$\begin{aligned}\partial_\lambda^2 \varepsilon \;=\; & (1/N)\sum_{ij}\left\{Tr\left[\left(\partial_\lambda^2 U\left(i,j\right)\right)\rho_{ij}\right]\right.\\ & \left.+\,Tr\left[\left(\partial_\lambda U\left(i,j\right)\right)\partial_\lambda \rho_{ij}\right]\right\},\end{aligned} \tag{2}$$

where ρ_{ij} is the reduced two-particle density operator and $U(i,j)$ includes all the single and two-body terms of the Hamiltonian associated with particles i and j. Now, assuming that $U(i,j)$ is a smooth function of the Hamiltonian parameters and that ρ_{ij} is finite at the critical point, *the origin of the discontinuity in the energy (discontinuity in or divergence of the first derivative of the energy) is the fact that one or more of the elements of* ρ_{ij} ($\partial_\lambda \rho_{ij}$) *are discontinuous (divergent) at the transi-*

tion point $\lambda = \lambda_c$ [7]. Since the concurrence and the negativity are both linear functions of the elements of ρ_{ij} it turns out that a discontinuity/divergence in one of them (in the derivative of one of them) implies a discontinuity/divergence of the energy (in the derivative of the energy) and vice-versa [7]. A natural question then arises: Does a ME measure show the same feature? In what follows, we give an explicit affirmative answer to this question [8].

In [6] three of us introduced two new quantities, both of which can be seen as generalizations of the Meyer-Wallach [14] Global Entanglement, originally defined for a system of N parties (particles). The first one is the average linear entropy of all $N_1 < N$ particles, where we assume a fixed "distance" between the N_1 particles. The second quantity is an average over all possible distances/configurations in which the N_1 particles can be arranged [6, 13]. For $N_1 = 1$ both quantities are the same ($G(1) = E_G^{(1)}$) and we recover the Meyer-Wallach measure. The first non-trivial case appears when $N \geq 4$ and we pick two particles ($N_1 = 2$) labeled by i and j. Now for a density matrix $\rho_{j,j+n}$ of dimension d we have $G(2,n) = \frac{d}{d-1}\left[1-(1/(N-n))\sum_{j=1}^{N-n} Tr\left(\rho_{j,j+n}^2\right)\right]$, which is the mean linear entropy of all pairs of particles $n = |i-j|$ sites apart, i.e., the mean entanglement between these pairs and the remaining $N-2$ particles. Averaging over all possible distances $1 \leq n < N$, $E_G^{(2)} = \frac{2}{N(N-1)}\sum_{n=1}^{N-1}(N-n)G(2,n)$. In order to simplify the notation (with no loss of generality), from now on we will work with the linear entropy of a single pair of particles n sites apart, which we call $\mathcal{G}(2,n)$. Note that in this notation $G(2,n) = \overline{\mathcal{G}(2,n)}$, being the average of $\mathcal{G}(2,n)$ over all particles n sites apart. For a translationally symmetric system $G(2,n) = \mathcal{G}(2,n)$.

Considering $\mathcal{G}(2,n)$ as a function of the tuning parameter λ we can write it and its derivative in terms of the lm elements of ρ_{ij} ($[\rho_{j,j+n}]_{lm}$) as

$$\mathcal{G}(2,n) = \frac{d}{d-1}\left[1-\sum_{l,m=1}^{d^2}\left|[\rho_{j,j+n}]_{lm}\right|^2\right], \quad (3)$$

$$\partial_\lambda \mathcal{G}(2,n) = \frac{2d}{1-d}\sum_{l,m=1}^{d^2}\left|[\rho_{j,j+n}]_{lm}\right|\partial_\lambda\left|[\rho_{j,j+n}]_{lm}\right|. \quad (4)$$

Therefore, since a discontinuity in one or more $[\rho_{j,j+n}]_{lm}$ *signals a 1QPT, a discontinuity in* $\mathcal{G}(2,n)$ *also signals a 1QPT. If* $\mathcal{G}(2,n)$ *is continuous and* $\partial_\lambda \mathcal{G}(2,n)$ *shows a discontinuity or divergence, it signals a 2QPT.* In this sense $\mathcal{G}(2,n)$ is at least as good as the concurrence/negativity to signal a QPT. Note that the previous result is valid only if the discontinuous/divergent quantities do not accidentally all vanish or cancel with other terms in Eqs. (3) and (4) (assumptions (b) and (c) in Ref. [7]). An added bonus of our approach, however, is that we do not need a further assumption, as in Ref. [7], related to the artificial/accidental divergences due to the maximization/minimization processes appearing in the definitions of the concurrence and the negativity. Moreover, $\mathcal{G}(2,n)$ is richer than the concurrence/negativity for signaling and classifying the order of a QPT, since it can be employed for the derivation of an EL, as we now demonstrate.

We particularize our discussion to two-level (qubit) systems [1]. In this case $\mathcal{G}(2,n)$ is written as

$$\mathcal{G}(2,n) = \frac{4}{3}\left[1-\frac{1}{4}\sum_{\alpha,\beta=0}^{3}\langle\sigma_j^\alpha\sigma_{j+n}^\beta\rangle^2\right], \quad (5)$$

where σ_i^α, $\alpha = 1,2,3$, are the Pauli operators and σ_i^0 is the identity. Thus, *as any measure dependent only on the two-particle reduced density matrix*, $\mathcal{G}(2,n)$ is *completely* determined by one- and two-point CFs. Whenever the system undergoes a second-order symmetry-breaking QPT, it will be reflected in one or more CFs and hence in the behavior of $\mathcal{G}(2,n)$. If the dominant (less rapidly decaying) CF decays with a power law ($\langle\sigma_i^{\alpha_0}\sigma_j^{\beta_0}\rangle \sim n^{-\eta}$) at the critical point (implying a diverging correlation length) and exponentially in its vicinity ($\langle\sigma_i^{\alpha_0}\sigma_j^{\beta_0}\rangle \sim e^{-n/\xi_C}$), so will $\mathcal{G}(2,n)$ increase. For large n, $\mathcal{G}(2,n) \approx \mathcal{G}(2,\infty) - \langle\sigma_i^{\alpha_0}\sigma_j^{\beta_0}\rangle^2/3$. Hence, close to the critical point $\mathcal{G}(2,n) \approx \mathcal{G}(2,\infty) - Ce^{-2n/\xi_C}$, where C is a constant, and $\mathcal{G}(2,n)$ increases exponentially fast, saturating for $n \gg \xi_C/2$. We can then define an EL that is proportional to the correlation length, $\xi_E = \xi_C/2$. The EL also diverges at the critical point with the same exponent as ξ_C, such that $\xi_E \sim |\lambda-\lambda_c|^{-\nu}$. At $\lambda = \lambda_c$, for large n, $\mathcal{G}(2,n) \approx \mathcal{G}(2,\infty) - C'n^{-2\eta}$, where C' is a constant. $\mathcal{G}(2,n)$ now increases as a power law with a power that is twice the CF exponent. Thus, $\mathcal{G}(2,n)$ inherits all the universal properties of the CFs. Moreover, due to the $\mathcal{G}(2,n)$ scaling with n, at the critical point the entanglement is more *distributed* in the system (any two spins are entangled with the rest of the chain) than away from it, indicating ME [3] prevails at the critical point. We emphasize that this result is quite general, applying to any collection of two-level systems with a second-order symmetry-breaking QPT. Next, we particularize to two specific cases in order to illustrate our general results.

For an arbitrary spin-1/2 model presenting a 1QPT, at least one of the CFs is discontinuous at the transition point. Thus, it is intuitive that $\mathcal{G}(2,n)$ is also discontinuous. A simple example is the *frustrated two-leg spin-1/2 ladder* discussed in Refs. [7, 15], where all but the $\langle\sigma_i^\alpha\sigma_j^\alpha\rangle$, $\alpha = x,y,z$, and $\langle\sigma_i^z\rangle$ expectation values vanish. The latter are discontinuous at the transition point but constant otherwise. The transition is clearly of first order and $\mathcal{G}(2,n)$ is able to signal it.

The one-dimensional XY model in a transverse mag-

netic field is described by the following Hamiltonian

$$H = -\sum_{i=1}^{N}\left\{\frac{J}{2}\left[(1+\gamma)\,\sigma_i^x\sigma_{i+1}^x + (1-\gamma)\,\sigma_i^y\sigma_{i+1}^y\right] + h\sigma_i^z\right\}, \tag{6}$$

where N is the total number of spins (sites) and $\gamma > 0$ is the anisotropy. This Hamiltonian is symmetric under a global π rotation about the z axis ($\sigma_i^{x(y)} \to -\sigma_i^{x(y)}$), implying a zero magnetization in the x or y directions ($\langle\sigma_i^{x(y)}\rangle = 0$). However, as the magnetic field h is decreased (or J increased) this symmetry is spontaneously broken at $\lambda = J/h = 1$ (in the thermodynamical limit) and a doubly-degenerate ground state with finite magnetization ($\pm M$) in the x direction develops, characterizing a ferromagnetic phase. It is possible then to define a symmetric ground state (with $\langle\sigma_i^x\rangle = 0$) as a superposition of these two degenerate ones. These states are of no use in practice, however, as they do not exist in real macroscopic objects undergoing a phase transition ("clustering property"). We call non-symmetric or broken-symmetry states the ones in which there is a finite magnetization ($\langle S_i^x = \sigma_i^x/2\rangle = \pm M$). Note that at the paramagnetic phase there is no such distinction. By further decreasing the magnetic field, a second phase transition occurs at $\gamma^2 + h^2 = 1$. In this "third" phase the approach of the CFs to their saturation values is not monotonic but oscillatory [16]. We should also say that this model reduces to the Ising model for $\gamma = 1$, where only the first critical point exists, and to the XX model as $\gamma \to 0$. However, the XX model belongs to a different universality class and we consider here only $0 < \gamma \leq 1$ [16].

The XY model can be solved exactly and all the CFs are known [16]. To calculate $\mathcal{G}(2,n)$ all we need is the one and two-point CFs (See Eq. (5)). Due to the translational invariance of the model ρ_{ij} depends only on the distance $n = |i-j|$ between the spins and $\langle\sigma_i^\alpha\sigma_j^\beta\rangle = \langle\sigma_j^\alpha\sigma_{j+n}^\beta\rangle = p_n^{\alpha\beta}$. Remembering that ρ_{ij} is Hermitian and has a unitary trace we are left with nine independent elements of ρ_{ij}, which may be functions of at most nine one- and two-point CFs. This number can be further reduced by the symmetries of the problem. The global symmetry under a π rotation about the z axis yields $\langle\sigma^{x(y)}\rangle = \langle\sigma_i^x\sigma_i^y\rangle = \langle\sigma_i^x\sigma_i^z\rangle = \langle\sigma_i^y\sigma_i^z\rangle = 0$ in the paramagnetic phase ($\lambda \leq 1$). We end up with four elements: $\langle\sigma^z\rangle$ and $\langle\sigma_i^\alpha\sigma_i^\alpha\rangle$, $\alpha = x, y, z$. In the ferromagnetic phase ($\lambda > 1$) this no longer holds since the Hamiltonian symmetry is not preserved by the ground state and we need to evaluate the nine one and two-point CFs. The four CFs appearing in the paramagnetic phase and $\langle\sigma_i^{x(y)}\rangle$ plus the three off-diagonal two-point ones were calculated in Ref. [16]. The first two $p_n^{yz} = p_n^{xy} = 0$ for all values of γ and λ [16]. The last off-diagonal CF (p_n^{xz}) was obtained exactly in terms of complex integrals whose calculation is cumbersome. However, we were able to obtain excellent bounds for it by imposing the positivity of the eigenvalues of ρ_{ij} [13].

With all the necessary CFs in hand $\mathcal{G}(2,n)$ for the XY model reads $\mathcal{G}(2,n) = 1-\frac{1}{3}[2\langle\sigma_j^x\rangle^2 + 2\langle\sigma_j^z\rangle^2 + 2\langle\sigma_j^x\sigma_{j+n}^z\rangle^2 + \langle\sigma_j^x\sigma_{j+n}^x\rangle^2 + \langle\sigma_j^y\sigma_{j+n}^y\rangle^2 + \langle\sigma_j^z\sigma_{j+n}^z\rangle^2]$. In Fig. 1 we plot the lower and upper bounds for $\mathcal{G}(2,1)$ (by using the upper and lower bounds of p_n^{xz}, respectively) as a function of λ and for a few γ's. We first note that it is maximal at the critical point for any anisotropy (this is true throughout the interval $0 < \gamma \leq 1$). Secondly, the bounds obtained are very tight and can barely be distinguished for some anisotropies. Only in the ferromagnetic phase and for $\gamma \to 0$ do the bounds become distinguishable. The derivative of $\mathcal{G}(2,1)$ with respect to λ is depicted in Fig. 2 exhibiting, as expected, a divergence at the critical point.

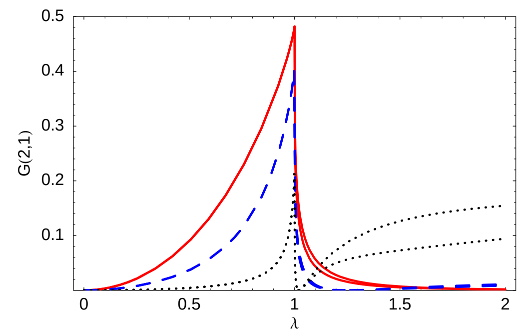

Figure 1: (Color online) Upper and lower bounds of $\mathcal{G}(2,1)$ for the XY chain for three values of the anisotropy: $\gamma = 1$ (red/solid), 0.6 (blue/dashed), and 0.2 (black/dotted).

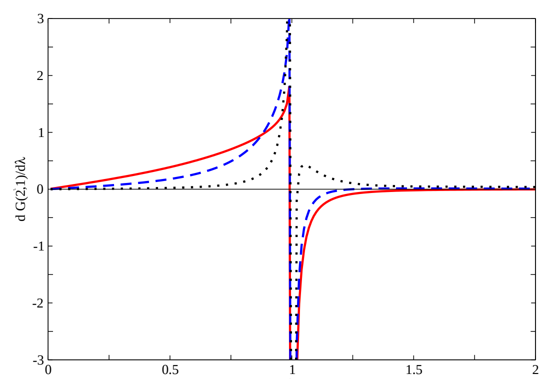

Figure 2: (Color online) Derivative of the lower bound of $\mathcal{G}(2,1)$ for three values of anisotropy: $\gamma = 1$ (red/solid), 0.6 (blue/dashed), 0.2 (black/dotted). The second phase transition is also imprinted for the $\gamma = 0.2$ as the curve crosses the abcissa at $\lambda = 1/\sqrt{1-\gamma^2}$.

Now we analyse how $\mathcal{G}(2,n)$ approaches its asymptotic value. It can be seen in Fig. 3 that $\mathcal{G}(2,n)$ is an increasing function of the distance n. To study this behavior analytically we make use of the asymptotic form of the CFs of the XY model: for $\lambda < 1$ [16], $\langle\sigma_j^x\sigma_{j+n}^x\rangle \sim n^{-1/2}\lambda_2^n$,

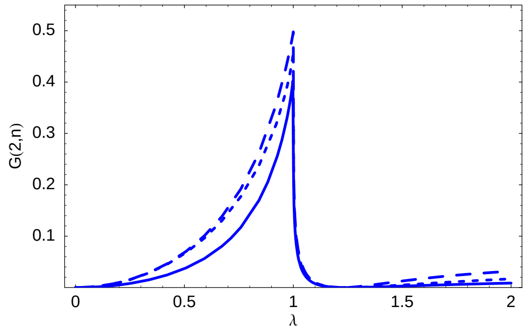

Figure 3: (Color online) Lower bound of $\mathcal{G}(2,n)$ for $\gamma = 0.6$ and for three values of n: $n = 1$ (solid), 2 (dashed), and 7 (long-dashed).

$\langle\sigma_j^y\sigma_{j+n}^y\rangle \sim n^{-3/2}\lambda_2^n$, and $\langle\sigma_j^z\sigma_{j+n}^z\rangle \sim \langle\sigma^z\rangle^2 - n^{-2}\lambda_2^{2n}$, with $\lambda_2 = (1/\lambda - \sqrt{1/\lambda^2 - (1-\gamma^2)})/(1-\gamma)$, while at the critical point $\langle\sigma_j^x\sigma_{j+n}^x\rangle \sim n^{-1/4}$, $\langle\sigma_j^y\sigma_{j+n}^y\rangle \sim n^{-9/4}$, and $\langle\sigma_j^z\sigma_{j+n}^z\rangle \sim \langle\sigma^z\rangle^2 - n^{-2}$. We can see from these expressions that, for large values of n, the dominant correlation is, as expected, in the x direction. Thus, for large n we can write $\mathcal{G}(2,n) \sim \mathcal{G}(2,\infty) - \langle\sigma_j^x\sigma_{j+n}^x\rangle^2/3$, such that

$$\mathcal{G}(2,n) \sim \mathcal{G}(2,\infty) - Cn^{-1}\lambda_2^{2n},\ \lambda < \lambda_c, \quad (7)$$

$$\mathcal{G}(2,n) \sim \mathcal{G}(2,\infty) - C'n^{-1/2}, \quad \lambda = \lambda_c. \quad (8)$$

From these expressions, we see explicitly that, at the critical point, the entanglement between two spins n sites apart increases as a power law of their distance, whereas away from the critical point it increases exponentially and saturates very fast. For the XY model the EL defined before reads $\xi_E = \frac{\gamma}{2(1-\lambda)}$, where we have used that $\lambda_2 \approx 1 + (\lambda-1)/\gamma$ near the critical point. Note that ξ_E diverges at the critical point as expected and that the ratio between ξ_E and the correlation length ξ_C is fixed: $\xi_E/\xi_C = 1/2$. Thus at the critical point the entanglement in the XY model is more distributed in the chain, as already indicated by the block entanglement [5].

In conclusion, we related the non-analytic properties of the ground state energy to the non-analyticities of $\mathcal{G}(2,n)$ for an arbitrary many-particle system. Thus, $\mathcal{G}(2,n)$ is able to signal both the quantum phase transition (QPT) points and the order of the transtition. $\mathcal{G}(2,n)$ is a multipartite entanglement (ME) measure which, for many reasons [13], is operationally good. Since no maximization/minimization process is needed for its calculation, no accidental discontinuities or divergences will occur (in contrast to the concurrence or the negativity). Moreover, for two-level systems $\mathcal{G}(2,n)$ is simply related to one- and two-point correlation functions (CFs). Therefore, for those systems undergoing a second order QPT it is possible to define a critical exponent and an entanglement length which is half the more familiar correlation length. We have exemplified those results with an explicit calculation for the XY transverse field spin-1/2 chain. This result adds strength to the conjecture by T. J. Osborne and M. A. Nielsen [3] that at the critical point bipartite entanglement (as given by the concurrence/negativity) is not maximal due to entanglement sharing, since all the parties involved are entangled as the entanglement length diverges. In fact, what should be maximal and favored is the *multipartite* entanglement, as we have plenty demonstrated. It is worth mentioning that any knowledge of the behavior of ME can only be achieved via the generalized global entanglement (GGE) and not by any CF alone. We expect that these findings will contribute to the understanding of the relevance of entanglement, specially ME, in QPTs.

Note: After this work was completed we became aware of an independent derivation of the entanglement length for the XY model in terms of the two-site *von Neumann entropy* [17]. We point out, however, that the relatively simple form of $\mathcal{G}(2,n)$, as given by the one and two-point CFs, allows it to be employed for the determination of the order of the QPT as well as for the derivation of an entanglement length for an arbitrary two-level system undergoing a second order QPT.

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